



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:52 PM GMT

PDB ID : 1YPF
Title : Crystal Structure of GuaC (BA5705) from Bacillus anthracis at 1.8 Å Resolution
Authors : Grenha, R.; Levnikov, V.M.; Blagova, E.V.; Fogg, M.J.; Brannigan, J.A.; Wilkinson, A.J.; Wilson, K.S.; Structural Proteomics in Europe (SPINE)
Deposited on : 2005-01-31
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

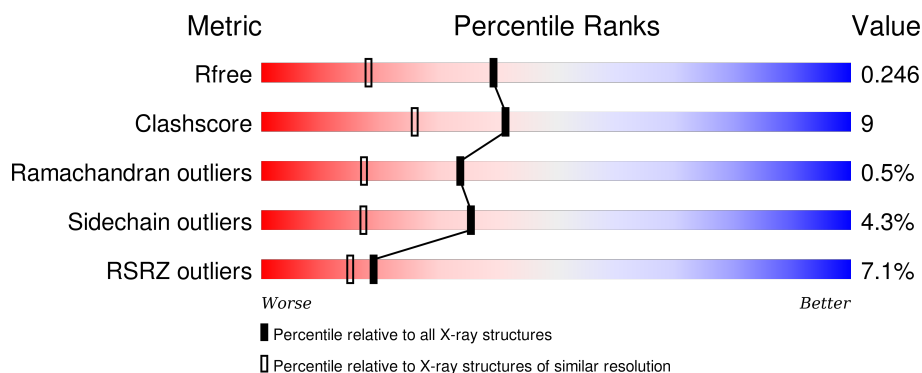
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	336	
1	B	336	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5246 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called GMP reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	3	0
			2285	1446	390	437	12			
1	B	295	Total	C	N	O	S	0	1	0
			2279	1441	390	436	12			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	CLONING ARTIFACT	UNP Q81JJ9
A	-7	SER	-	CLONING ARTIFACT	UNP Q81JJ9
A	-6	SER	-	CLONING ARTIFACT	UNP Q81JJ9
A	-5	HIS	-	CLONING ARTIFACT	UNP Q81JJ9
A	-4	HIS	-	CLONING ARTIFACT	UNP Q81JJ9
A	-3	HIS	-	CLONING ARTIFACT	UNP Q81JJ9
A	-2	HIS	-	CLONING ARTIFACT	UNP Q81JJ9
A	-1	HIS	-	CLONING ARTIFACT	UNP Q81JJ9
A	0	HIS	-	CLONING ARTIFACT	UNP Q81JJ9
B	-8	GLY	-	CLONING ARTIFACT	UNP Q81JJ9
B	-7	SER	-	CLONING ARTIFACT	UNP Q81JJ9
B	-6	SER	-	CLONING ARTIFACT	UNP Q81JJ9
B	-5	HIS	-	CLONING ARTIFACT	UNP Q81JJ9
B	-4	HIS	-	CLONING ARTIFACT	UNP Q81JJ9
B	-3	HIS	-	CLONING ARTIFACT	UNP Q81JJ9
B	-2	HIS	-	CLONING ARTIFACT	UNP Q81JJ9
B	-1	HIS	-	CLONING ARTIFACT	UNP Q81JJ9
B	0	HIS	-	CLONING ARTIFACT	UNP Q81JJ9

- Molecule 2 is water.

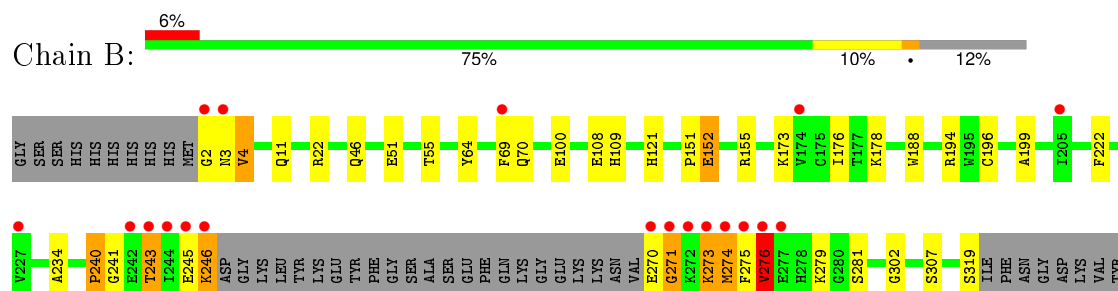
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	311	Total	O	0	0
			311	311		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	371	Total	O	0	0
			371	371		

- Molecule 1: GMP reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α , β , γ	114.68Å 114.68Å 52.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.85 – 1.80 29.85 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.85-1.80) 99.8 (29.85-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.174 , 0.238 0.188 , 0.246	Depositor DCC
R_{free} test set	3225 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.690	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 72.8	EDS
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	3 of 63559 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5246	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.66	0/2334	0.73	1/3152 (0.0%)
1	B	0.73	1/2322 (0.0%)	0.70	0/3133
All	All	0.70	1/4656 (0.0%)	0.72	1/6285 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	TYR	CD1-CE1	-5.14	1.31	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	ARG	NE-CZ-NH1	8.64	124.62	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	222	PHE	Peptide
1	A	268	ASN	Peptide
1	B	240	PRO	Peptide
1	B	271	GLY	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2285	0	2297	35	0
1	B	2279	0	2285	43	0
2	A	311	0	0	14	0
2	B	371	0	0	19	0
All	All	5246	0	4582	78	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (78) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:GLU:O	1:B:246:LYS:HB2	1.51	1.06
1:B:100:GLU:HG3	2:B:555:HOH:O	1.64	0.94
1:B:273:LYS:HB3	1:B:276:VAL:O	1.66	0.94
1:B:196:CYS:SG	2:B:687:HOH:O	2.28	0.92
1:B:51:GLU:HG3	2:B:527:HOH:O	1.73	0.89
1:A:269:VAL:HG11	2:A:555:HOH:O	1.73	0.87
1:A:279:LYS:HD2	2:A:524:HOH:O	1.76	0.85
1:B:108:GLU:HB3	2:B:634:HOH:O	1.74	0.85
1:B:246:LYS:O	1:B:270:GLU:HB3	1.82	0.79
1:B:4:VAL:HB	2:B:603:HOH:O	1.85	0.76
1:A:236:HIS:CD2	2:A:524:HOH:O	2.37	0.76
1:B:273:LYS:CB	1:B:276:VAL:O	2.35	0.74
1:B:274:MET:O	1:B:275:PHE:HB2	1.87	0.73
1:A:242:GLU:H	1:A:275:PHE:HE1	1.38	0.71
1:B:108:GLU:O	1:B:109:HIS:HB2	1.90	0.71
1:B:276:VAL:HG22	2:B:686:HOH:O	1.90	0.71
1:A:45:MET:SD	2:A:500:HOH:O	2.51	0.68
1:B:234:ALA:O	1:B:279:LYS:HD2	1.95	0.67
1:A:276:VAL:HG11	2:A:625:HOH:O	1.93	0.67
1:A:79:ARG:HD2	2:A:441:HOH:O	1.94	0.66
1:A:273:LYS:HG3	1:A:277:GLU:HA	1.78	0.66
1:A:178:LYS:HE2	2:A:452:HOH:O	1.97	0.64
1:B:243:THR:HB	1:B:274:MET:HG2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:HIS:HD2	2:B:337:HOH:O	1.83	0.61
1:B:51:GLU:O	1:B:55:THR:HG23	2.01	0.60
1:A:121:HIS:HD2	2:A:344:HOH:O	1.84	0.60
1:A:242:GLU:O	1:A:274:MET:O	2.20	0.59
1:A:320:ILE:C	2:A:328:HOH:O	2.40	0.59
1:A:274:MET:O	1:A:275:PHE:HD1	1.85	0.59
1:A:187:GLY:N	2:A:401:HOH:O	2.29	0.58
1:A:236:HIS:HE1	1:A:285:THR:OG1	1.87	0.57
1:B:178:LYS:HE2	2:B:473:HOH:O	2.04	0.56
1:B:4:VAL:HG12	2:B:391:HOH:O	2.06	0.56
1:B:194:ARG:HD2	1:B:222:PHE:CD1	2.40	0.56
1:B:4:VAL:CG1	2:B:391:HOH:O	2.55	0.55
1:B:246:LYS:O	1:B:270:GLU:N	2.40	0.55
1:B:155:ARG:HE	1:B:199:ALA:HB1	1.73	0.54
1:A:269:VAL:HG12	1:A:270:GLU:H	1.73	0.53
1:A:236:HIS:CE1	1:A:285:THR:OG1	2.62	0.53
1:A:274:MET:O	1:A:275:PHE:CD1	2.62	0.52
1:B:246:LYS:O	1:B:270:GLU:CB	2.56	0.51
1:A:194:ARG:HH11	1:A:194:ARG:HG3	1.76	0.51
1:A:159:ASN:HB3	2:A:584:HOH:O	2.10	0.51
1:A:272:LYS:O	1:A:273:LYS:HD2	2.11	0.50
1:B:2:GLY:N	2:B:539:HOH:O	2.45	0.49
1:B:245:GLU:O	1:B:246:LYS:CB	2.37	0.49
1:A:276:VAL:CG1	2:A:625:HOH:O	2.59	0.49
1:B:196:CYS:N	2:B:687:HOH:O	2.45	0.49
1:B:194:ARG:HH11	1:B:222:PHE:HD1	1.60	0.49
1:A:3:ASN:HB2	2:A:442:HOH:O	2.12	0.48
1:B:22:ARG:NH1	2:B:495:HOH:O	2.46	0.48
1:A:273:LYS:HG3	1:A:277:GLU:CA	2.44	0.48
1:B:46:GLN:HG2	2:B:402:HOH:O	2.13	0.47
1:A:148:VAL:HG11	1:A:157:LEU:HD22	1.96	0.47
1:A:111:THR:HG21	1:A:140:GLU:HB2	1.96	0.47
1:B:151:PRO:HD3	2:B:687:HOH:O	2.14	0.47
1:B:108:GLU:O	1:B:109:HIS:CB	2.62	0.47
1:A:276:VAL:O	1:A:277:GLU:CB	2.63	0.47
1:A:269:VAL:HG12	1:A:270:GLU:N	2.30	0.46
1:B:279:LYS:NZ	2:B:510:HOH:O	2.46	0.46
1:A:22:ARG:HD3	1:A:295:SER:OG	2.14	0.46
1:B:69:PHE:CD2	1:B:70:GLN:HG3	2.51	0.46
1:A:7:TYR:CE1	1:A:190:LEU:HD13	2.51	0.46
1:B:302:GLY:HA3	1:B:307:SER:OG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ARG:CG	1:A:194:ARG:HH11	2.29	0.45
1:A:319:SER:HA	2:A:438:HOH:O	2.16	0.44
1:B:246:LYS:H	1:B:270:GLU:N	2.15	0.44
1:B:11:GLN:NE2	2:B:352:HOH:O	2.49	0.44
1:B:240:PRO:HA	1:B:241:GLY:HA2	1.75	0.43
1:B:307:SER:OG	2:B:559:HOH:O	2.21	0.43
1:B:270:GLU:CG	1:B:271:GLY:N	2.81	0.43
1:A:175:CYS:O	1:A:179:ILE:HG12	2.19	0.43
1:A:273:LYS:HG3	1:A:277:GLU:H	1.84	0.42
1:B:194:ARG:HD3	2:B:553:HOH:O	2.19	0.42
1:A:13:ILE:HD11	1:A:314:VAL:HG13	1.99	0.42
1:B:152[B]:GLU:CD	1:B:152[B]:GLU:H	2.05	0.41
1:B:4:VAL:HG23	1:B:188:TRP:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	294/336 (88%)	280 (95%)	12 (4%)	2 (1%)	26	11
1	B	292/336 (87%)	277 (95%)	14 (5%)	1 (0%)	46	29
All	All	586/672 (87%)	557 (95%)	26 (4%)	3 (0%)	34	17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	269	VAL
1	A	276	VAL
1	B	276	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	249/280 (89%)	239 (96%)	10 (4%)	38	20
1	B	246/280 (88%)	233 (95%)	13 (5%)	28	11
All	All	495/560 (88%)	472 (95%)	23 (5%)	35	15

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	118[A]	ASP
1	A	118[B]	ASP
1	A	155	ARG
1	A	194	ARG
1	A	270	GLU
1	A	274	MET
1	A	276	VAL
1	A	277	GLU
1	A	281	SER
1	B	3	ASN
1	B	4	VAL
1	B	152[A]	GLU
1	B	152[B]	GLU
1	B	173	LYS
1	B	176	ILE
1	B	243	THR
1	B	246	LYS
1	B	273	LYS
1	B	274	MET
1	B	276	VAL
1	B	281	SER
1	B	319	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	11	GLN
1	A	121	HIS
1	A	236	HIS
1	B	3	ASN
1	B	11	GLN
1	B	104	GLN
1	B	121	HIS
1	B	318	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	295/336 (87%)	0.38	23 (7%) 16 12	17, 28, 55, 73	0
1	B	295/336 (87%)	0.17	19 (6%) 23 18	16, 24, 49, 74	0
All	All	590/672 (87%)	0.27	42 (7%) 19 15	16, 26, 53, 74	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	269	VAL	11.9
1	A	276	VAL	10.3
1	B	244	ILE	10.0
1	B	275	PHE	8.4
1	B	242	GLU	7.0
1	A	275	PHE	7.0
1	A	244	ILE	6.9
1	B	276	VAL	6.5
1	B	245	GLU	6.4
1	A	274	MET	6.1
1	B	271	GLY	5.9
1	A	277	GLU	5.7
1	A	270	GLU	5.6
1	B	2	GLY	5.5
1	A	268	ASN	5.5
1	B	274	MET	5.3
1	B	270	GLU	5.2
1	A	320	ILE	5.0
1	A	271	GLY	4.9
1	A	242	GLU	4.8
1	A	243	THR	4.8
1	A	69	PHE	3.9
1	A	109	HIS	3.7
1	B	277	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	243	THR	3.2
1	B	246	LYS	3.1
1	A	106	ALA	3.1
1	A	3	ASN	3.0
1	B	69	PHE	2.9
1	A	273	LYS	2.8
1	B	227	VAL	2.8
1	A	107	ALA	2.7
1	A	41	VAL	2.7
1	B	205	ILE	2.6
1	B	174	VAL	2.6
1	B	272	LYS	2.5
1	B	273	LYS	2.5
1	A	235	GLY	2.4
1	B	3	ASN	2.3
1	A	96	GLU	2.3
1	A	272	LYS	2.2
1	A	23	SER	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.